https://doi.org/10.33805/2641-7383.128
Volume 4 Issue 1 | PDF 128 | Pages 2

EDELWEISS PUBLICATIONS
OPEN ACCESS

Edelweiss Chemical Science Journal

Editorial ISSN: 2641-7383

Beyond the Scope of Each Computational Chemistry

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Citation: Akitsu T, Suda S and Katsuumi N. Beyond the scope of each computational chemistry (2021) Edelweiss Chem Sci J 4: 25-26.

Received: Sep 06, 2021
Accepted: Sep 18, 2021
Published: Sep 22, 2021

Abstract

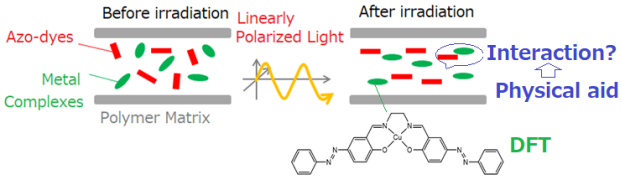
Due to recent advances in computational chemistry, not only computers and analysis programs in crystal structure analysis, but also TD-DFT calculations related to intramolecular electronic states and energies have been easily performed, and detailed discussions have become possible. On the other hand, how to discuss information such as intermolecular interactions, molecular assembly states, and packing, which is beyond the scope of application of each computational chemistry program and theory, is still a subject of research. Here, authors would like to consider what is possible and difficult using a program, for example, Hirshfeld surface analysis.

Keywords: Crystal structure analysis, Hirshfeld surface analysis, TD-DFT, Intermolecular interaction, Hybrid materials

Abbreviations: TD-DFT-Time Dependent-Density Functional Theory

Introduction

With the aid of computational chemistry, current coordination chemistry has developed to reach deep understanding such as optimized structures, electronic structures (simulated spectra), and reactivity based on thermodynamic energy. In particular, DFT calculation provides detailed information of metal complexes including organic ligands as well as metal ions. Besides intramolecular information, however, coordination chemists may also be interested in intermolecular effects of hybrid materials or photochemistry or spectroscopy associated with spatially asymmetric conditions to discuss their metal complexes. One of the ways to overcome such situations may be to employ conventional physical frameworks based on the DFT results for molecular information (**Scheme 1**), which was proposed by us in certain international conference.



Scheme 1: Concept of one of hybrid approaches of DFT and physical principle for dipole-dipole interaction.

In recent years, calculations for crystal structure analysis of small molecule compounds have generally been performed relatively smoothly by well-developed programs, from various data processing programs to theoretical calculations for discussion using results. In fact, in our laboratory, we examined whether it is possible to discuss the coordination bond of metal complexes by comparing the electron density by experiment with the electron density by TD-DFT theoretical calculation using a conventional program [1].

Results and Discussion

With the ultimate goal of expressing the antibacterial activity of the novel hydrazone ligand complex, we are conducting docking simulations with proteins based on crystal structure analysis data, and are studying intermolecular interactions between ligands and proteins. Focusing on molecular recognition by ligands outside the complex molecule, crystal structure analysis (re-determination) of Nicotinohydrazide derivative hydrazone with only a ligand having a new structure and intermolecular mutual as crystals by Hirshfeld surface analysis compared with similar compounds containing different solvents (**Figure 1**) or isomers at the pyridine site [2-6] (**Figure 2**).

In order to visualize the intermolecular interactions in the crystal of the compounds, a Hirshfeld surface analysis was performed with a CrystalExplorer 17.5 program. The fingerprint plot for this structure shows typical wings. The percentage contribution of each intermolecular interaction to the Hirshfeld surface area is shown in the figures. Hirshfeld surface analysis is a computational method that discusses intermolecular interactions in the case of a single compound that forms a molecular crystal. Except for the method of forming molecular crystals, that is, the conformation that is the most stable in terms of energy and the prediction of crystal packing. It must be still a difficult problem.

Various ligand-protein docking calculation programs are known for intermolecular interactions between small molecule compounds and other substances. The basis is the crystal structure of proteins and ligands and the DFT-optimized structure of ligands. It has the meaning of simplifying complicated factors in order to evaluate the contribution of shape and various interactions as one numerical value called "docking score". On the other hand, similar discussions are difficult for organic-inorganic nanocomposites whose three-dimensional structure is undecided. For example, is it possible to use the description of curved surfaces using mathematics of differential geometry to express only the shape?

Furthermore, is it possible to discuss the hydrophobic / hydrophilic interaction with a solvent (around the dielectric environment) in solution by diverting the donor or acceptor of the potential interaction by Hirshfeld surface analysis? Should ordinary physical laws be used in addition to the knowledge of computational chemistry to consider interactions with surfactants and solvent micro-spaces (nano-droplets, etc.)?

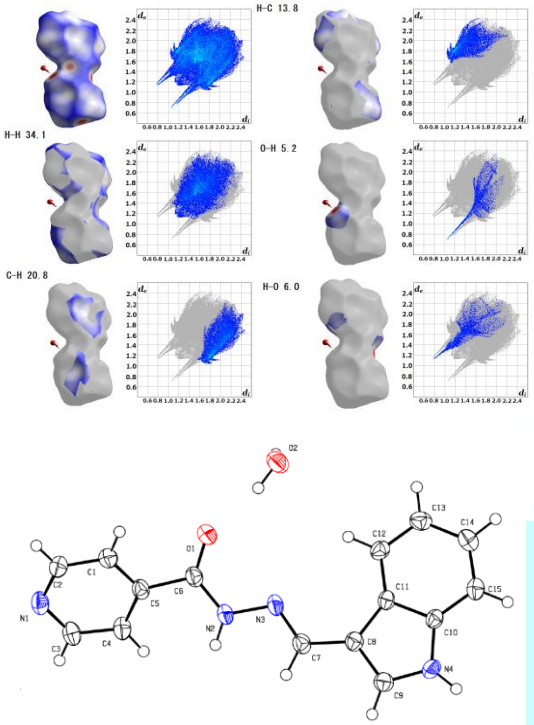


Figure 1: Hirshfeld surface analysis of $C_{15}H_{12}N_4O.H_2O$ [2].

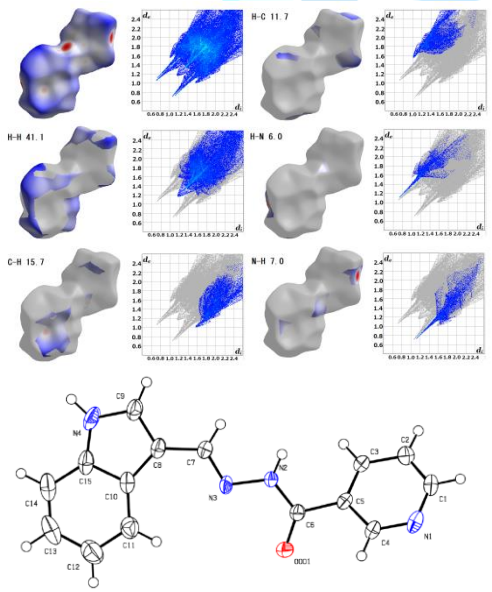


Figure 2: Hirshfeld surface analysis and ORTEP drawing of $C_{15}H_{12}N_4O$ [6].

Conclusion

While simple analytical calculations and computational theoretical chemistry have become widespread, it is another matter whether or not to discuss all substances of interest today. Of course, high-precision computational chemistry has a range of applications. It may be less accurate, but humans may apply the laws of physics (using computational chemistry data) to consider it.

Acknowledgement

This work was supported by a Grant-in-Aid for Scientific Research (A) KAKENHI (20H00336). The authors thank Prof. Emmanuel N. N for at Department of Chemistry, University of Buea for suggestion of hydrazone compounds.

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